WHAT IS CLAIMED IS:

1. A method for validating a computer modeling of a molecular system, said method comprising

selecting a model parameter of said molecular system;

selecting a validation measure of said molecular system;

simulating said molecular system by said computer modeling with said selected model parameter;

then determining a value of said validation measure of said molecular system from said simulating step; and

testing whether said value of said validation measure is in a predetermined range to validate said computer modeling.

2. The method of claim 1, wherein the model parameter is rigidity of a bond formed between two atoms in the molecular system.

3. The method of claim 1, wherein the model parameter is a bond length or bond angle between two atoms in the molecular system.

4. The method of claim 1, wherein the model parameter is temperature or pressure of the molecular system.

5. The method of claim 1, wherein the model parameter is the identity of an atom or group of atoms in the molecular system.

6. The method of claim 1, wherein the model parameter is the charge on an atom in the molecular system.

7. The method of claim 1, wherein the validation measure is selected from the group consisting of a force between atoms in the molecular system, a bond length or angle between atoms of the molecular system, shape of the molecular system, binding affinity between components of the molecular system, and velocity of atoms of the molecular system.

8. The method of claim 1, wherein the model parameter is rigidity of a bond between atoms in the molecular system, the validation measure is a force acting on the atoms,

and the predetermined range is a range of forces compatible with a rigid bond between the atoms.

9. The method of claim 1, further comprising synthesizing a compound component of the molecular system,determining a value of the validation measurement for the synthesized compound, and comparing the value for the synthesize compound to value of the validation measure for the molecular system.

10. The method of claim 1, further comprising

varying said model parameter of said molecular system;

simulating said molecular system by said computer modeling with said varied model parameter;

then redetermining said value of said validation measure of said molecular system from said simulating step; and

retesting whether said redetermined value of said validation measure is in a predetermined range to validate said computer modeling.

11. The method of claim 10, wherein model parameter is charge of an atom of the molecular system, the validation measure is a binding affinity between compound and target components of the molecular system, one of which contains the atom, the predetermined range is a range of binding affinities, and the varying step varies the magnitude of the charge on the atom.

12. The method of claim 10, wherein the model parameter is temperature, the validation measure is velocity of atoms of the molecular system, the predetermined range is a range of velocities, and the varying step varies the temperature of the model system.

13. The method of claim 10, wherein the model parameter is identity of an amino acid in a protein component of the molecular system, the validation measure is a binding affinity of the protein component for a target component of the molecular system, the predetermined range is a range of binding affinities, and the varying step varies the identity of the amino acid.

14. The method of claim 13, wherein the varying step varies the identity of the amino acid by a conservative substitution.

15. The method of claim 13, wherein the varying step varies the identity of the amino acid by a nonconservative substitution.

16. The method of claim 10, wherein said varying, simulating, redetermining and retesting steps are performed iteratively.

17. The method of claim 10, wherein in said varying step said model parameter is varied discretely.

18. The method of claim 10, wherein in said varying step said model parameter is varied continuously.

19. A method for validating a computer modeling of a molecular system, said method comprising

selecting a model parameter of said molecular system;

selecting a validation measure of said molecular system;

simulating said molecular system by said computer modeling with said selected model parameter;

then determining a value of said validation measure of said molecular system from said simulating step;

varying said model parameter of said molecular system;

resimulating said molecular system by said computer modeling with said varied model parameter;

then redetermining a value of said validation measure of said molecular system from said simulating step; and

calculating a derivative from a change in said validation measure with respect to a change in said model parameter;

testing whether said derivative is in a predetermined range to validate said computer modeling.

20. A method for validating a computer modeling of a molecular system, said method comprising

selecting a model parameter of said molecular system;

selecting a validation measure of said molecular system;

simulating said molecular system by said computer modeling with said selected model parameter;

then determining a first result of said validation measure of said molecular system from said simulating step; and

varying the model parameter of the molecular system

simulating said molecular system by said computer modeling with said varied model parameter;

determining a second result of said validation measure of said molecular system from said simulating step;

determining whether the difference between the first and second results is expected from the variation in the validation measure.